CLAIMS

What is claimed is:

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1. A method of characterizing spectrometer instruments according to instrumental variation, comprising the steps of:

providing standard spectral measurements from at least one spectrometer instrument; and

classifying said spectral measurements into predefined clusters on the basis of extracted spectral features; and

providing calibration models for each of said predefined clusters, wherein said calibration model compensates for said instrumental variation.

15 2. The method of Claim 1 wherein said instrumental variation comprises any of:

wavelength shifts;

nonlinear wavelength shifts;

wavelength expansions;

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wavelength contractions;

nonlinear wavelength expansions;

source intensity drifts;

blackbody profile changes;

bandwidth changes;

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resolution changes;

baseline deviations;

changes over time;

temperature effects;

detector response;

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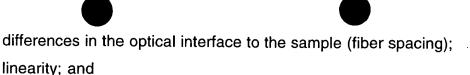
differences in optical components (e.g. long-pass filters or fiber optics);

variation related to mounting of references;

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rule.



detector cut-off.

- 5 3. The method of Claim 1, wherein said standard spectra are measured on a plurality of spectrometer instruments.
 - 4. The method of Claim 1, wherein said standard spectral are measured on a single spectrometer instruments at successive time intervals.
 - 5. The method of Claim 1, wherein said classifying step comprises the steps of:
 extracting features; and
 classifying said features according to a classification model and decision
 - 6. The method of Claim 5, wherein said feature extraction step comprises any mathematical transformation that enhances a particular aspect or quality of data that is useful for interpretation.
 - 7. The method of Claim 3, wherein said classification model comprises means for determining a set of similarity measures with predefined classes.
- 8. The method of Claim 5, wherein said decision rule comprises means for assigning class membership on the basis of a set of measures calculated by a decision engine.
 - 9. The method of Claim 4, wherein individual features are divided into two categories, said categories comprising:
- abstract wherein said features are extracted using various computational methods; and

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simple features that are derived from an *a priori* understanding of a system, wherein said feature is directly related to an instrument parameter or component.

5 10. The method of Claim 7, wherein said abstract features are calculated using any of:

plotting primary principal components versus one another and identifying resulting clusters;

discrminant anlysis; and

10 k-means clustering.

11. The method of Claim 5, wherein said classification step further comprises the step of employing factor-based methods to build a model capable of representing variation in a measured spectrum related to variations in spectral response;

wherein projection of a measured absorbance spectrum onto said model constitutes a feature that represents spectral variation related to instrument variation.

20 12. The method of Claim 5, wherein said classifying step further comprises the steps of:

measuring the similarity of a feature to predefined clusters; and assigning membership in a cluster.

- 25 13. The method of Claim 5, further comprising the step of: assigning measurements in an exploratory data set to clusters.
 - 14. The method of Claim 13, further comprising the step of:
 using measurements and class assignments to determine a mapping from features to cluster assignments.

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15. The method of Claim 13, further comprising the steps of:

defining clusters from said features in a supervised manner, wherein each set of features is divided into two or more regions, and wherein classes are defined by combinations of feature divisions;

designing a classifier subsequent to class definition through supervised pattern recognition by determining an optimal mapping or transformation from the feature space to a class estimate which minimizes the number of misclassifications; and

creating a model based on class definitions which transforms a measured set of features to an estimated classification.

- 16. The method of Claim 1, further comprising the step of providing calibration models for analysis of new sample measurements.
- 15 17. The method of Claim 16, wherein said calibration models model differences between said predefined clusters.
 - 18. The method of Claim 16, wherein a master calibration model is developed for a first of said clusters from a set of exemplar spectra with reference values and pre-assigned classification definitions.
 - 19. The method of Claim 18, further comprising the step of transferring said master calibration model to a plurality of slave calibration models, wherein a slave calibration model is calculated for each remaining cluster, and wherein a transform modifies said master calibration model to a slave calibration model in accordance with principal features defining each of said classes.
- 20. The method of Claim 19, wherein said transferring step comprises the steps of:

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transferring said master calibration model to a first slave calibration model;

transferring said first slave calibration model to a second slave calibration model;

and repeating said transfer from one slave calibration model to another slave calibration model, until a calibration has been provided for each of said predefined clusters;

wherein a transform modifies said transferred calibration models in accordance with principal features defining each of said clusters.

- 21. The method of Claim 18, further comprising the step of transferring said master calibration model to a plurality of slave calibration models, wherein a slave calibration model is calculated for each remaining cluster, and wherein a transform modifies said slave calibration model to said master calibration model in accordance with principal features defining each of said classes.
- 22. The method of Claim 21, wherein said transferring step comprises the steps of:

transferring said master calibration model to a first slave calibration model;

transferring said first slave calibration model to a second slave calibration model;

and repeating said transfer from one slave calibration model to another slave calibration model, until a calibration has been provided for each of said predefined clusters;

wherein a transform modifies said transferred calibration models in accordance with principal features defining each of said clusters.

23. The method of Claim 16, wherein a different calibration model is developed for each class, and wherein said calibration models are developed

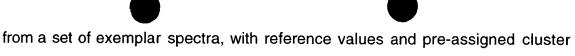
definitions.

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- 24. The method of Claim 23, wherein a spectrum is assigned to one of many predefined clusters for which a calibration model has been developed.
 - 25. The method of Claim 1, further comprising the steps of: providing new spectral measurements;

comparing said new spectral measurements to each of said pre-defined clusters according to extracted spectral features;

reporting those measurements as outliers for which a matching cluster is not found.

26. A method of developing calibration models for spectral analysis comprising the steps of:

defining clusters from an exemplar data set of spectral measurements, wherein said clusters exhibit a high degree of internal similarity;

mapping said clusters to one another, wherein principal features distinguishing clusters from one another are determined;

calculating a calibration model for a first of said clusters, said calibration model comprising a master calibration;

transferring said master calibration to at least one slave calibration, wherein a slave calibration comprises a calibration derived by applying a transform to slave spectra such that the master calibration now models the difference between the master cluster and another cluster corresponding to said slave spectra.